



# The Diffusion-Brusselator Equation

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(Received September 1994; accepted October 1994)

**Abstract**—A solution is found for the reaction-diffusion equation, called the diffusion-Brusselator equation [1] using the decomposition method.

The problem of dealing with chemical reactions of systems involving two variable intermediates, together with a number of initial and final products whose concentrations are assumed to be controlled throughout the reaction process is an important one under quite realistic conditions and is discussed by Nicolis and Prigogine in [1]. It is necessary to consider at least a cubic nonlinearity in the rate equations [2]. This model has been referred to as the trimolecular model or Brusselator [3]. It represents a useful model for study of cooperative processes in chemical kinetics. Such a trimolecular reaction step arises in the formation of ozone by atomic oxygen via a triple collision. It arises also in enzymatic reactions, and in plasma and laser physics in multiple couplings between certain modes.

The development of the decomposition method [4] makes possible not only the solution of the Brusselator but extensions to general models with wide classes of nonlinearities. No linearization or perturbation is necessary, so much more realistic solutions are obtained than were previously possible.

The equation is given in the form [5]

$$\begin{aligned}\frac{\partial u}{\partial t} &= B + u^2v - (A + 1)u + \alpha \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \\ \frac{\partial v}{\partial t} &= Au - u^2v + \alpha \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right).\end{aligned}$$

The problem [1] states initial conditions  $u(0, x, y) = 2 + 0.25y$ ,  $v(0, x, y) = 1 + 0.8x$ ,  $A = 3.4$ ,  $B = 1$ ,  $\alpha = 0.002$ , and Neumann boundary conditions  $\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0$  where  $u$  and  $v$  are chemical concentrations of reaction products,  $A$  and  $B$  are constant concentrations of input reagents, and  $\alpha$  is a constant based on a diffusion coefficient and a reactor length.\*

Writing  $L_t$  for  $\frac{\partial}{\partial t}$  and operating on both sides of the equations  $L_t^{-1}(\cdot) = \int_0^t (\cdot) dt$ , we have

$$\begin{aligned}u &= u(0, x, y) + L_t^{-1}B + L_t^{-1}u^2v - L_t^{-1}(A + 1)u + L_t^{-1}\alpha \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \\ v &= v(0, x, y) + L_t^{-1}Au - L_t^{-1}u^2v + L_t^{-1}\alpha \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right).\end{aligned}$$

This work was supported by the Atmospheric Sciences Laboratory (R. E. Meyers) under the auspices of the U.S. Army Research Office Scientific Services Program administered by Battelle.

\*See the discussion on parallel methods for O.D.E.'s in reference [1].

Using decomposition [2], identify  $u(0, x, y)$  as  $u_0$  and  $v(0, x, y)$  as  $v_0$  in the decompositions of  $u$  into  $\sum_{n=0}^{\infty} u_n$  and  $v$  into  $\sum_{n=0}^{\infty} v_n$ . The nonlinearity  $u^2v$  is written as  $\sum_{n=0}^{\infty} A_n$  where the  $A_n$  are the Adomian polynomials generated for  $u^2v$ .

By the decomposition method [2],

$$\begin{cases} u_0 = u(0, x, y) + L_t^{-1}B \\ v_0 = v(0, x, y) \\ \begin{cases} u_1 = L_t^{-1}A_0\{u^2v\} - L_t^{-1}(A+1)u_0 + L_t^{-1}\alpha\left(\frac{\partial^2}{\partial x^2}u_0 + \frac{\partial^2}{\partial y^2}u_0\right) \\ v_1 = L_t^{-1}Au_0 - L_t^{-1}A_0\{u^2v\} + L_t^{-1}\alpha\left(\frac{\partial^2}{\partial x^2}v_0 + \frac{\partial^2}{\partial y^2}v_0\right) \end{cases} \\ \vdots \\ \begin{cases} u_m = L_t^{-1}A_{m-1}\{u^2v\} - L_t^{-1}(A+1)u_{m-1} + L_t^{-1}\alpha\left(\frac{\partial^2}{\partial x^2}u_{m-1} + \frac{\partial^2}{\partial y^2}u_{m-1}\right) \\ v_m = L_t^{-1}Au_{m-1} - L_t^{-1}A_{m-1}\{u^2v\} + L_t^{-1}\alpha\left(\frac{\partial^2}{\partial x^2}v_{m-1} + \frac{\partial^2}{\partial y^2}v_{m-1}\right) \end{cases} \end{cases}$$

The  $A_n\{u^2v\}$  can be written using algorithms given in the literature (see, for example, [2] or [3]). For convenience of the reader, we list

$$\begin{aligned} A_0 &= u_0^2v_0 \\ A_1 &= 2u_0u_1v_1 \\ A_2 &= (u_1^2 + 2u_0u_2)v_2 \\ A_3 &= (2u_0u_3 + 2u_1u_2)v_3 \\ A_4 &= (u_2^2 + 2u_1u_3 + 2u_0u_4)v_4 \\ &\vdots \end{aligned}$$

Hence, the decomposition components  $u_0, u_1, \dots$  and  $v_0, v_1, \dots$  are determinable, and we write the approximants  $\varphi_m[u] = \sum_{n=0}^{m-1} u_n$  and  $\varphi_m[v] = \sum_{n=0}^{m-1} v_n$  which converge to  $u$  and  $v$ , respectively. Such solutions have been shown to become quite accurate within a few terms [2–9].

In the operator format of decomposition [3], we have

$$\begin{aligned} Lu &= g + R_1u + N(u, v), \\ Lv &= R_2u + R_3v - N(u, v). \end{aligned}$$

Let  $g = 1$ ,  $R_1 = \frac{22}{5} + \frac{1}{500}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$ ,  $R_2 = \frac{17}{5}$ ,  $R_3 = \frac{1}{500}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$ ,  $N(u, v) = u^2v$ ,  $L = \frac{\partial}{\partial t}$ , and  $L^{-1} = \int_0^t (\cdot) dt$ .

The solution is found in terms of the components

$$\begin{cases} u_0 = 2 + \frac{1}{4}y + L^{-1}[1] \\ u_{n+1} = L^{-1}R_1u_n + L^{-1}A_n(u_0, \dots, u_n; v_0, \dots, v_n) \\ \begin{cases} v_0 = 1 + \frac{4}{5}x \\ v_{n+1} = L^{-1}R_2u_n + L^{-1}R_3v_n - L^{-1}A_n(u_0, \dots, u_n; v_0, \dots, v_n) \end{cases} \end{cases}$$

for  $n \geq 0$ . Then  $u = \sum_{n=0}^{\infty} u_n$  and  $v = \sum_{n=0}^{\infty} v_n$  are approximated by  $\varphi_m[u] = \sum_{n=0}^{m-1} u_n$  and  $\varphi_m[v] = \sum_{n=0}^{m-1} v_n$ .

(The problem is solvable also as a boundary-value problem by solving for the highest-order linear terms in  $x$  or  $y$ , and defining the inverse operators as two-fold indefinite integrations as discussed in [2]. This is more difficult because of the stiffness and the Neumann conditions which must be matched to each successive approximant  $\varphi_1, \varphi_2, \dots, \varphi_m$ .)

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